Kondo effect in transport through Aharonov-Bohm and Aharonov-Casher interferometers

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Abstract

We derive the extension of the Hubbard model to include Rashba spin-orbit coupling that correctly describes Aharonov-Bohm and Aharonov-Casher phases in a ring under applied magnetic and electric fields. When the ring is connected to conducting leads, we develop a formalism that is able to describe both, Kondo and interference effects. We find that in the Kondo regime, the spin-orbit coupling reduces strongly the conductance from the unitary limit. This effect in combination with the magnetic flux, can be used to produce spin polarized carriers.

1. Introduction

There is a great interest in nanoscopic systems, either because of its potential application in nanodevices or as ideal systems to test theories for non-trivial physical problems. In particular, the Kondo effect is present in many of these systems, like magnetic impurities on clean noble metal surfaces or quantum corrals [1], small clusters on these surfaces [2,3] and systems of quantum dots [4,5,6,7,8,9]. In particular, the unitary limit, which consists in the maximum possible conductance through a quantum dot has been reached experimentally [4]. The Kondo model out of equilibrium brings new challenges to the theory [10,11].

On the other hand, effects of interference in quantum paths and the Aharonov-Bohm effect have been demonstrated in mesoscopic rings with embedded quantum dots [4,5,12,13].

The calculation of transport through a mesoscopic ring in which both interference effects and interactions leading to the Kondo effect are present is not trivial. An example of this is a recent debate about the role of interactions in dephasing [14]. Even knowing the exact eigenstates of the ring, there is no simple procedure to calculate the conductance. When the coupling V of the ring to the conducting leads is small, using perturbation theory up to second order in V, an expression has been derived, which is also exact for any V in the non-interacting limit, the Jagla-Balseiro formula [15]. Similar equations were used recently [16,17]. Alternative perturbative expressions were also proposed [18]. Unfortunately these expressions are not valid in the Kondo regime, in which the ground state of the isolated ring is Kramers degenerate (odd number of electrons), because the ground state of the whole system is a singlet with a characteristic energy scale (the Kondo temperature) $T_K \sim W \exp[-1/\rho_0 J]$, where W is the band width, ρ_0 the density of states at the Fermi level and $J \approx V^2$ [see Eq. (12) or Ref. [3]], which cannot be recovered by perturbation theory in V. Previous calculations of the conductance through strongly correlated rings in which the effects of interference were important to detect signatures of spin-charge separation, assumed that a Zeeman term destroys the Kondo effect in the system [16]. For a ring described by the ionic Hubbard model, it has been shown that the conductance through the system is related to the quasiparticle weight [17]. The physics of the Kondo regime was recovered by mapping the model into an impurity Anderson model, but at the cost of losing interference effects.

One of the branches of nanophysics with particular recent interest is spintronics, which consists in developing means of creating and controlling spin polarized currents in nanoscale systems [19]. An important ingredient for this

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purposes is the Rashba spin-orbit coupling

$$H_{\mathrm{SOC}} = \alpha \vec{\sigma} \cdot \vec{\mathrm{E}} \times (\vec{\mathrm{p}} - e\vec{\mathrm{A}}), \tag{1}$$

which is present in quantum wells. Recent experiments in semiconductor mesoscopic rings have shown that the conductance oscillates not only as a function of the applied magnetic field (Aharonov-Bohm effect) but also as a function of the applied electric field $\vec{\mathrm{E}}$ perpendicular to the plane of the ring (Aharonov-Casher effect) [21,22]. In this effect, the electrons, as they move, capture a phase that depends on the spin, as a consequence of spin-orbit coupling. The main features of the experiment can be understood in a one-electron picture [23,24]. However, this picture is inadequate in the presence of strong correlations. In particular, the Kondo effect cannot be described.

The aim of the present work is two-fold: first, to provide a method to calculate the conductance through a ring that is able to capture at the same time the Kondo physics and interference effects; second, to apply the formalism to calculate the conductance through a ring under the action of both, magnetic and electric fields together with Rashba spin-orbit coupling H_{SOC}. In the second task we stumbled with the difficulty of finding the form of the Hubbard model in the presence of H_{SOC}, which adequately describes the periodicity with the applied electric field seen in the experiments. We solved this problem using a non-abelian gauge transformation in the continuum version of the model, which translates the effect of H_{SOC} to a change in the boundary conditions.

The main physical result is that the combination of both Kondo effect and spin-orbit coupling leads to a strongly spin dependent conductivity that might be used for spin filtering purposes. Some results have been recently published [25]. In section 2 we briefly explain the general method to calculate the conductance. In section 3, the Hubbard model including the effect of the spin-orbit coupling Eq. (1) is derived. Section 4 contains results for a four-site ring. Section 5 is a summary and discussion.

2. Formalism to calculate the conductance

To calculate the conductance through an interacting subsystem, it is necessary to obtain some Green functions of the whole system, which includes the interacting part both leads [26]. An example of an interferometer assembled experimentally with one quantum dot is given in Fig. 1 of Ref. 5. The Hamiltonian can be written as

$$H = H_I + H_l + H_V$$
$$H_I = H'_U - V_g \sum_{i\sigma} d^\dagger_{i\sigma} d_{i\sigma},$$

$$H_l = t_c \left(\sum_{i=0,\sigma}^{-\infty} c^\dagger_{i-1,\sigma} c_{i\sigma} + \sum_{i=1,\sigma}^{\infty} c^\dagger_{i+1,\sigma} c_{i\sigma} + \mathrm{H.c} \right),$$

$$H_V = V \left(\sum_\sigma c^\dagger_{0\sigma} d_{0\sigma} + c^\dagger_{1\sigma} d_{1\sigma} + \mathrm{H.c.} \right). \tag{2}$$

H_I describes the interacting subsystem (in the case described below, a Hubbard ring with spin-orbit coupling). The operator $d^\dagger_{i\sigma}$ creates an electron with spin σ at site i in this subsystem. The second term of H_I represents the effect of a gate voltage. The term H_l describes both leads, and H_V is the coupling between both leads and the interacting region. We label the sites in this region so that site 0 is coupled to the left lead and site 1 to the right one. The prime in H'_U reminds us that the Hamiltonian of the subsystem is written in a particular gauge, as described in the next section. Note that the phases of all $c_{i\sigma}$ operators can be chosen so that t_c and V are real, regardless of the above mentioned gauge. The Zeeman term is neglected here. To reduce the number of parameters, we have assumed identical left and right leads and the same coupling between any of them and the interacting subsystem.

Since H_I describes a finite system, it can be diagonalized exactly. Our general approach to calculate the conductance amounts to a truncation of the Hilbert space of H_I, retaining only two neighboring charge configurations, with n and $n-1$ particles. It can be shown that this procedure is valid for small enough V [8]. Calculating the matrix elements of H_V in the truncated Hilbert space leads to a generalized Anderson model

$$H_{\mathrm{GAM}} = H_l + \sum_{n,j} E^n_{j\sigma} |\psi^n_j\rangle\langle\psi^n_j|$$
$$+ V \sum_{\eta k, j\sigma} (\beta^\eta_{kj\sigma} c^\dagger_{\eta\sigma} |\psi^{n-1}_k\rangle\langle\psi^n_j| + \mathrm{H.c.}), \tag{3}$$

where $|\psi^n_j\rangle$ and E^n_j denote the j-th eigenvector and eigenvalue of H_I in the configuration with n particles and

$$\beta^\eta_{kj\sigma} = \langle\psi^{n-1}_k|d_{\eta\sigma}|\psi^n_j\rangle \quad (\eta = 0,1). \tag{4}$$

In the simplest case, only the spin singlet (doublet) ground state of H_I is relevant for the configuration with an even (odd) number of electrons and H_{GAM} reduces to the ordinary Anderson model [17]. However, interference effects, for example the vanishing of the conductance through the ring for certain values of the flux [16] is a consequence of an *orbital* degeneracy of levels for that flux and more states than one Kramers doublet should be included in H_{GAM}, as we report in section 4.

In general, H_{GAM} can be represented using one or more slave bosons that represent the relevant eigenstates of H_I with an even number of particles [27,28]. A model with a doublet hybridized with a singlet and a triplet has been solved using the numerical renormalization group [29]. From the solution of H_{GAM}, the conductance is obtained using known expressions that relate it with the exact Green functions of H_{GAM} [26].

3. Hubbard model in the presence of spin-orbit interaction

The simplest way to add the physics of the spin-orbit coupling in the Hubbard model seems to be to replace H_{SOC}

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given by Eq. (1) by a tight-binding version in which the current in each link is multiplied by the Pauli matrix perpendicular to the link and to the electric field, to build the cross product of Eq. (1) [30]. For an electric field in the z direction and a ring in the x, y plane this gives:

$$H_{tb} = \alpha E_z \hbar/(2a) \sum_i [i \cos\varphi (d_{i+1\uparrow}^\dagger d_{i\downarrow} + d_{i+1\downarrow}^\dagger d_{i\uparrow})$$
$$+ \sin\varphi (d_{i+1\uparrow}^\dagger d_{i\downarrow} - d_{i+1\downarrow}^\dagger d_{i\uparrow}) + \text{H.c.}]. \tag{5}$$

However, in the experimentally assembled *rings* it is clear that the conductance *oscillates* as $\vec{E}$ increases [21,22] and therefore one expects that the electric field enters an exponential as a phase, and this is not apparent in Eq. (5).

To follow a procedure that leads to such an exponential dependence, we consider the version of the model in the continuum H_U^c. This is obtained from the noninteracting version derived by Meijer *et al.* [31] for electric and magnetic fields perpendicular to the plane of the ring, adding a local interaction. The Hamiltonian is

$$H_U^c = \hbar\Omega \sum_j \left[-i\frac{\partial}{\partial\varphi_j} - \frac{\phi}{\phi_0} + \frac{\gamma}{2}\sigma_r(\varphi_j) \right]^2$$
$$+ U \sum_{i<j} \delta(\varphi_i - \varphi_j), \tag{6}$$

where φ_j is the azimuth of the j-th electron, $\Omega = \hbar/(2m^*r^2)$, m^* is the effective electron mass, r is the radius of the ring, $\gamma = \alpha E_z/(r\Omega)$ is proportional to the Rashba constant α and the electric field E_z, $\phi = B\pi r^2$ is the magnetic flux, $\phi_0 = hc/e$ is the flux quantum and $\sigma_r(\varphi) = \sigma_x \cos\varphi + \sigma_y \sin\varphi$ is the Pauli matrix in the radial direction.

It can be easily checked that the unitary transformation $T = \prod_j t(\varphi_j)$, with

$$t(\varphi) = \exp\left[-i\sigma_z\frac{\varphi}{2}\right] \exp\left[i\vec{\sigma}.\vec{n}_\theta\frac{\varphi'}{2}\right] \exp\left[i\frac{\phi}{\phi_0}\varphi\right],$$
$$\vec{n}_\theta = (-\sin\theta, 0, \cos\theta), \theta = \arctan(\gamma),$$
$$\varphi' = \varphi\sqrt{1+\gamma^2}, \tag{7}$$

makes the dependence of the fields [ϕ and γ in Eq. (6)] disappear in the transformed Hamiltonian $H_U^{c\prime} = T^\dagger H_U^c T$. Therefore $H_U^{c\prime}$ is the continuum version of the ordinary Hubbard model, in which the magnetic flux and the spin-orbit coupling have been gauged away. The price to pay is that the transformed one-particle spinors satisfies the boundary conditions $\chi'(2\pi) = t^\dagger(2\pi)\chi'(0)$ (instead of periodic ones). This implies that in the Hubbard model for a ring of N sites, the last hopping (from angle $\varphi = -2\pi/N$ to 0) should be modified. Diagonalizing $T^\dagger(2\pi)$ one obtains the eigenvalues $\exp[i(\Phi_{AB} + \sigma\Phi_{AC})]$, where $\sigma = \pm 1$ for spin pointing in the $\pm\vec{n}_\theta$ direction, $\Phi_{AB} = 2\pi\phi/\phi_0$, and $\Phi_{AC} = \pi\{[1+\gamma^2]^{1/2} - 1\}$.

Then, the transformed Hubbard model for a ring of N sites takes the form

$$H_U' = -\sum_{i=0,\sigma}^{N-2} t \left[d_{i+1\sigma}^\dagger d_{i\sigma} + \text{H.c.} \right]$$
$$- t \left[e^{i(\Phi_{AB} + \sigma\Phi_{AC})} d_{0\sigma}^\dagger d_{N-1,\sigma} + \text{H.c.} \right]$$
$$+ U \sum_i d_{i\uparrow}^\dagger d_{i\uparrow} d_{i\downarrow}^\dagger d_{i\downarrow}, \tag{8}$$

where

$$\Phi_{AC} = \sqrt{\pi^2 + R^2} - \pi, \tag{9}$$

and the ratio $R = \pi\gamma$ is given by $\hbar\alpha E_z N/(2ta)$ if the mass is eliminated from the curvature of the bottom of the non-interacting band ($m^* = \hbar^2/(2ta^2)$, where $a = 2\pi r/N$ is the lattice parameter). If instead $m^* = \hbar k_F/v_F$ is used, where k_F, v_F are the Fermi wave vector and velocity respectively

$$R = \frac{\hbar\alpha E_z N k_F a}{2ta\sin(k_F a)}. \tag{10}$$

In any case, the same qualitative physics is described. The rotational invariance of H_U' can be recovered replacing $d_{j\sigma}^\dagger = \tilde{d}_{j\sigma}^\dagger \exp[i(\Phi_{AB} + \sigma\Phi_{AC})j/N]$.

It is important to remark that the spin quantization axis of Eq. (8) varies with position. For $\varphi = 0$ (corresponding to $y = 0$), it is given by $\vec{n}_\theta$ (see Eq. (7)) and it lies in the x, z plane. For other angles the spin quantization axis rotates with φ in such a way that the component in the plane of the ring (x, y) always points towards the center of the ring.

It is interesting to note that Berry phases captured in adiabatic evolutions of a system in Φ_{AB} and Φ_{AC} give information on the polarization, opening of a spin gap, phase transitions and ferrotoroidic moments [32,33].

4. Results for 4-site ring

For the explicit calculation, we take a ring of $N = 4$ sites, connected to the leads at opposite sites, lying at $\phi = 0$ and $\phi = \pi$. We assume that the leads are described by a constant density of states $\rho_0 = 1/W$ and set the band width $W = 60t$ (much larger than the hopping t in the ring). The Fermi energy of the leads is set at the on-site energy in the ring (zero). We have included all doublet states with $n = 3$ and the singlet ground state for $n = 4$ of H_I, to construct the generalized Anderson model H_{GAM} (see Eq. (3)). We have solved H_{GAM} in a slave boson mean-field approximation, which is known to reproduce correctly the exponential dependence of the Kondo scale on the parameters. Details are given in Ref. [25].

4.1. The different regimes

The properties of the effective generalized Anderson model, Eq. (3) and therefore the conductance through the ring, differ according to different regimes which depend on the ratio of the charge-transfer energy $E_0^{(4)} - E_0^{(3)}$,
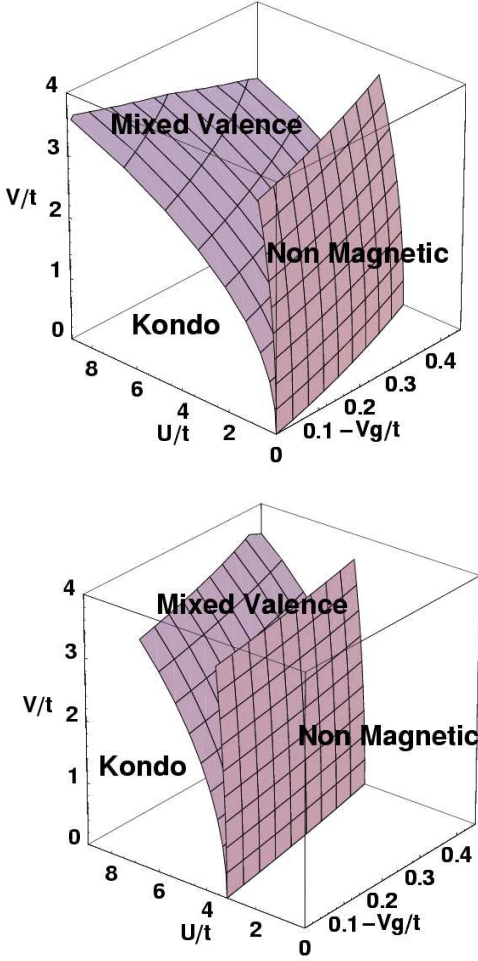
Fig. 1. Different regimes of the model for spin-orbit strength $R = 0$ and two values of the applied magnetic flux:$\Phi_{AB} = 0$ (top) and $\Phi_{AB} = \pi$ (bottom).

where $E_0^{(n)}$ is the ground state of H_I in the subspace of n electrons, and the effective resonant level width

$$\Delta = \pi \rho_0 V^2 \sum_\eta |\beta_{00\sigma}^\eta|^2. \tag{11}$$

If the four-particle singlet is well below the lowest Kramers doublet ($E_0^{(3)} - E_0^{(4)} \gg \Delta$) the system is in the non-magnetic regime. For increasing values of $E_0^{(4)}$, the system enters first the intermediate valence zone ($|E_0^{(3)} - E_0^{(4)}| \sim \Delta$), and then the Kondo regime when the lowest spin doublet is well below the singlet ($E_0^{(4)} - E_0^{(3)} \gg \Delta$).

In Fig. 1 we show the different regions of parameters of the model U, V_g and V (setting t as the unit of energy) corresponding to the different regimes in absence of spin-orbit coupling. The boundary between the mixed-valence regime and the nonmagnetic (Kondo) one has been defined arbitrarily in the figure by $E_0^{(3)} = E_0^{(4)} + \Delta$ ($E_0^{(3)} = E_0^{(4)} - 8\Delta$). Note that there is a strong dependence of the boundaries

with the applied magnetic flux. The four-particle singlet is favored for $\Phi_{AB} = \pi$. This can be understood already for the non-interacting ring, since the ground-state energy for four particles $E_0^{(4)}$ is optimized for $\Phi_{AB} = \pi$, while it passes through a relative maximum at $\Phi_{AB} = 0$. In the strongly interacting case $U \to +\infty$, H_U' reduces to a $t - J$ model and $E_0^{(4)}$ becomes independent of the flux, while $E_0^{(3)}$ is minimized for $\Phi_{AB} = 0$ [16].

Clearly, there is no mixed valence regime for $V = 0$, since this implies $\Delta = 0$, while the extension of this regime increases nearly quadratically with V.
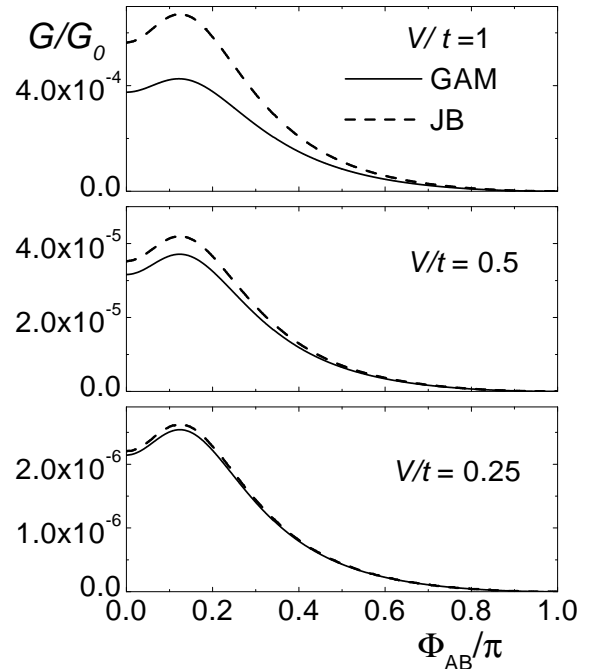
4.2. The non-magnetic regime

Fig. 2. Conductance as a function of magnetic flux for $R = 0$, $V_g = -0.8t$, $U = 2t$ and several values of V. Full lines: our formalism. Dashed lines: Jagla-Balseiro formula.

In Fig. 2 we show the conductance $G = G_\uparrow + G_\downarrow$ as a function of magnetic flux in the non-magnetic regime for different values of V and without applied electric field ($R = 0$). The quantum of conductance is denoted as $G_0 = 2e^2/h$. The total conductance is even with flux ϕ and we show G in the interval $0 < \phi < \phi_0/2$ (or $0 < \Phi_{AB} < \pi$).

The conductance is very small due to the fact that there are no available states of the ring near the Fermi energy. G increases with the hopping to the leads V, since this term promotes electrons to the leads at the Fermi level. In addition, in this regime correlations play a minor role and one expects that the Jagla-Balseiro formula [15], which is exact in the non-interacting case, gives accurate values for the conductance. In fact, our results show the same qualitative behavior and for small V it can be demonstrated that both

approaches are equivalent in this regime. However, there are significant quantitative differences for $V/t = 1$. It is difficult to state which approach is the most acurate in this case.

In absence of spin-orbit coupling, for an applied flux of half a flux quantum, the conductance vanishes due to destructive interference, as a consequence of reflection symmetry of the ring for a non-degenerate ground state [16].

4.3. *Spin dependent conductance in the Kondo regime*

In the rest of this paper, we consider $E_{0\sigma}^{(3)} < E_0^{(4)}$, when the ring is the mixed valence or Kondo regime. In Fig. 3 we show the conductance as a function of the applied magnetic flux Φ_{AB} for several values of the applied electric field E_z. We discuss first the case $E_z = R = 0$. In contrast to the results in the non-magnetic regime, the conductance takes appreciable values, being near to the ideal one for $0.2 < \Phi_{AB} < 0.5$ and $1.5 < \Phi_{AB} < 1.8$. The system can be considered to be in the Kondo regime for these values of Φ_{AB} and in the mixed valence regime for other fluxes. This is also consistent with the calculated occupation of the levels, shown elsewhere [25], which is nearly one in the Kondo regime. As expected from Fig. 1, the region of Φ_{AB} for which the system is in the Kondo regime increases with decreasing V, and for $V = 3.1t$ nearly perfect conductance is obtained for $0.1 < \Phi_{AB} < 0.7$ and $1.3 < \Phi_{AB} < 1.9$ [25]. This corresponds to the unitary limit. This limit, observed experimentally in systems with one quantum dot different than ours [4], is characteristic of the Kondo regime. The Jagla-Balseiro formula fails to describe this case, giving very small values of the conductance. Note that the conductance still vanishes at $\Phi_{AB} = \pi$ as a consequence of interference. This together with the ideal conductance for the Kondo regime shows that our approach includes both, interference and Kondo effects, in contrast to previous calculations [16,17].

Precisely in the Kondo regime, where the conductance reaches its maximum possible value, is where the effect of the spin-orbit coupling times the applied electric field E_z is most noticeable. As it can be seen in Fig. 3, moderate values of E_z are enough to decrease the conductance from G_0 to very small values. The main reason for this is that E_z affects both spin projections in opposite ways breaking SU(2) symmetry, and therefore tends to destroy the Kondo singlet. The stabilization energy of this singlet is of the order of the Kondo temperature

$$T_K \sim W \exp(-\pi(E_0^{(4)} - E_0^{(3)})/\Delta), \qquad (12)$$

and therefore decreases exponentially inside the Kondo regime. For the parameters of Fig. 3, the system is deeper in the Kondo regime for $\Phi_{AB} \sim \pm 0.3\pi$ (mod 2π). Due to the loss of reflection symmetry, in presence of spin-orbit
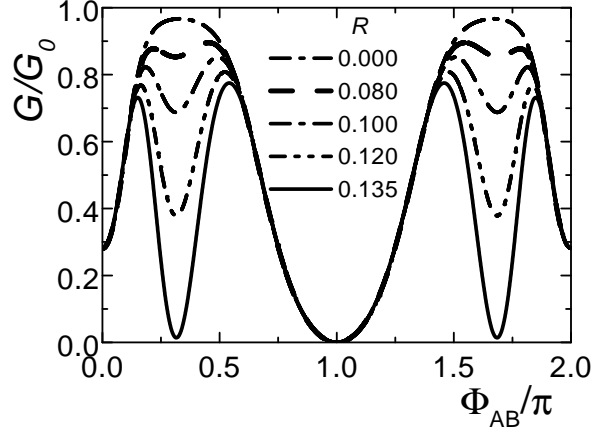

Fig. 3. Conductance as a function of flux for $V = 3.5t, V_g = 0, U = 6t$ and different values of the electric field times spin-orbit coupling strength R (see text).

coupling, complete conductance cancellation is not realized at $\Phi_{AB} = \pi$.

The above mentioned breaking of spin SU(2) symmetry as a consequence of the spin-orbit coupling leads to significant differences in the conductance G_σ for both spin orientations σ. Since in our Hamiltonian, the quantization axis depends on the position of the electron, this conductance should be interpreted in the following way: if a spin σ (up or down) in the quantization direction $\vec{n}_\theta = (-\sin\theta, 0, \cos\theta)$ (see Eq.(7)) is injected in the ring at the right lead ($\varphi = 0$) it comes out at the left lead ($\varphi = \pi$) with spin σ in the direction $\vec{n}'_\theta = (\sin\theta, 0, \cos\theta)$ or vice versa. For an arbitrary direction, the incident wave should be decomposed in the components along the corresponding quantization axis. In Fig. 4 we show the degree of polarization of the conductance $P = (G_\uparrow - G_\downarrow)/(G_\uparrow + G_\downarrow)$ as a function of Φ_{AB} for several E_z. The ratio $P = \pm 1$ at symmetric points near $\Phi_{AB} = \pi$ because one of the G_σ vanishes there and the other one at the symmetric point around π [the Hamiltonian is invariant under time reversal and change of sign of $\Phi_{AB} = 2(\pi r)^2 B/\phi_0$]. For fluxes corresponding to the Kondo regime $P \sim 0.4$ and one of the G_σ can still be near the ideal one.

5. Summary and discussion

We propose an approach to calculate the conductance through a ring of interacting quantum dots, weakly coupled to conducting leads, that takes into account both interference effects and non-perturbative many-body ones, mapping the relevant states into an effective generalized Anderson model containing several non-degenerate states. Here we have solved the model using a slave-boson representation in the saddle-point approximation, but alternative treatments like the numerical renormalization group are also possible.

We have derived an extension of the Hubbard model that includes spin-orbit interaction, absorbing it in op-
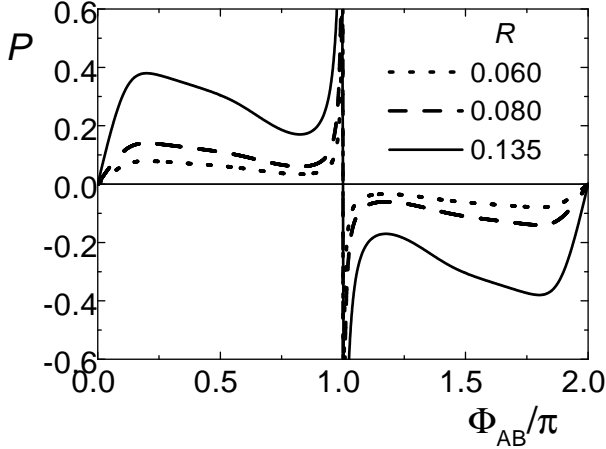
Fig. 4. Polarization of the conductance $P = (G_\uparrow - G_\downarrow)/(G_\uparrow + G_\downarrow)$ as a function of flux for $V = 3.5t$, $V_g = 0$, $U = 6t$ and different electric fields.

posite Aharonov-Casher phases for spin up and down in an adequately chosen quantization axis, defined by a non-abelian gauge transformation. For a non-interacting system, it has been noticed previously that the Rashba spin-orbit coupling can be gauged away in a ring [34], although the explicit dependence of the boundary conditions [the Aharonov-Casher phase Φ_{AC}, see Eq. (9)] with the applied electric field was not given. Using Bethe ansatz, the persistent currents in a Hubbard ring were calculated as a function of Φ_{AC} by Fujimoto and Kawakami [35]. These authors also note that the trick used to gauge away the spin-orbit coupling can be extended to any SU(2) invariant interactions (not only local as U). For example a nearest-neighbor repulsion $\sum_{i\sigma\sigma'} d^\dagger_{i+1\sigma} d_{i+1\sigma} d^\dagger_{i\sigma'} d_{i\sigma'}$ is not modified by a spin rotation at any site. Therefore, the thermodynamic properties of the extended Hubbard model including this interaction should not vary with spin-orbit coupling in the thermodynamic limit, in which boundary conditions are irrelevant. This fact is not obvious in alternative treatments [36].

We have calculated the conductance through a ring described by the Hubbard model with Rashba spin-orbit coupling in presence of magnetic and electric fields. The main effect of the spin-orbit coupling is to tend to destroy the Kondo effect, leading to a strong spin dependence of the conductance.

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